Solving three-body scattering problem in the momentum lattice representation

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A brief description of the novel approach towards solving few-body scattering problems in a finite-dimensional functional space of the L_2-type is presented. The method is based on the complete few-body continuum discretization in the basis of stationary wave packets. This basis, being transformed to the momentum representation, leads to the cell-lattice-like discretization of the momentum space. So the initial scattering problem can be formulated on the multi-dimensional momentum lattice which makes it possible to reduce the solution of any scattering problem above the breakup threshold (where the integral kernels include, in general, some complicated moving singularities) to convenient simple matrix equations which can be solved on the real energy axis. The phase shifts and inelasticity parameters for the three-body nd elastic scattering with MT I-III NN potential both below and above the three-body breakup threshold calculated with the proposed wave-packet technique are in a very good agreement with the previous accurate benchmark calculation results.

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1. Motivation of the work. The strictly proved integral equations for the solution of few-body scattering problems were developed many years ago by Faddeev and Yakubosky [1, 2]. After these pioneer works a lot of investigations in the few-body quantum physics have been done along these lines for a few last decades. In spite of a great progress in this field [3, 4, 5, 6, 7, 8, 9], the practical solution of the few-nucleon scattering problems with realistic $2N$- and $3N$- interactions, especially above the three body breakup threshold, is still remained rather cumbersome computational problem which needs an appeal to very powerful computer resources. Moreover, even till now $4N$ systems above the three-body threshold can be practically treated within the Faddeev–Yakubovsky framework only with simple pairwise local interactions [6, 9]. The reason is in very laborious numerical routines in the coordinate space or complicated moving singularities in kernels of the integral momentum-space equations.

At the same time, several efficient methods for the approximation of few-body continuum wavefunctions in various L_2 bases have been developed [10, 11, 12, 13, 14, 15, 16, 17, 18]. These are the "moment T-matrix method" [10], J-matrix approach [11, 12, 13], "the harmonic oscillator representation" [14], the Lorentz integral transform method [15], the continuum-discretized coupled-channel method (CDCC) [16, 17, 18] etc. However most of them can be used for special cases of the few-body scattering only, e.g. for the so called truly few-body scattering when there are no bound states in any two-body subsystems [14], or for the composite particle scattering off heavy target when stripping channels can be neglected [16, 17, 18]. In other cases one describes the processes when the few-body wavefunctions in the initial channel are of bound-state type and L_2 basis is used to approximate the final-state few-body continuum only [15], or one treats a three-body scattering at small energies below the three-body threshold only [13]. So that, with the above L_2-type methods no precise calculations for the basic three-body $n-d$ scattering case above the breakup threshold have been carried out up to date.[1]

Thus, it would be very convenient to have in our disposal a sufficiently universal method for general continuum discretization in different two- and few-body scattering problems (in nuclear, atomic, hadronic etc. physics), which operating with L_2 functions only and non-singular matrix equations both below and above the breakup thresholds.

Few years ago the present authors have developed a new approach to solving few-body scattering problems based on discretization of continuous spectrum of total Hamiltonian [20, 21, 22, 23, 24]. The method uses the stationary wave packets, i.e. are L_2-type functions, instead of the exact scattering wave functions. In these works an original wave-packet formalism have been developed which allowed to construct finite-dimensional (f.-d.) approximations for basic scattering-theory operators and find the scattering observables using such approximations. The approach have recently been tested for the elastic scattering and breakup of a composite projectiles scattered off heavy targets (with neglecting the stripping processes), and a perfect agreement with the CDCC method results have been found [23, 24]. In the present paper we extend our wave-packet approach much further, towards solving a general three-body scattering problem on the base of the projected Faddeev equations and illustrate it on example of quartet and doublet $n-d$ scattering

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[1] The realistic three-nucleon calculations for e.g. nd (or pd) scattering below and above three-body breakup threshold have been done either with variational method [19] using the Schrödinger equation approach or with the Faddeev equations in the momentum [8] or in the configuration space [5].

below and above three-nucleon breakup threshold[2].

2. Formulation of the approach. Here we describe the three-body wave-packet discretization procedure for the elastic $n-d$ scattering. The elastic amplitude X for the quartet case can be found from a single integral Faddeev equation [25]

$$X = -Pv_1 - Pv_1G_1X, \tag{1}$$

where v_1 is the triplet NN interaction potential, $G_1 = (E - H_1)^{-1}$ is the three-body resolvent of the channel Hamiltonian $H_1 = H_0 + v_1$ and P is the permutation operator.

Let us introduce some finite basis $\{|S_i\rangle\}_{i=1}^{\mathcal{N}}$ such that the projector $\Gamma_{\mathcal{N}}$ onto the f.-d. basis subspace can (in some not rigorous sense) approximate the unit operator $\Gamma_{\mathcal{N}} = \sum_{i=1}^{\mathcal{N}} |S_i\rangle\langle S_i| \to 1$. Then one can define the $\mathcal{N}$-dimensional approximation for any operator A as its projection onto the respective basis subspace: $\Gamma_{\mathcal{N}} A \Gamma_{\mathcal{N}} = \sum_{ij} |S_i\rangle A_{ij} \langle S_j|$, with corresponding matrix elements $A_{ij} \equiv \langle S_i|A|S_j\rangle$. Using such matrix approximations for the scattering operators, the initial integral equation can be reduced to the respective matrix equation. We will denote the matrices of projected operators with corresponding bold letters. So, one finds the matrix equation instead of the integral equation (1):

$$\mathbf{X} = -\mathbf{P}\mathbf{v}_1 - \mathbf{P}\mathbf{v}_1\mathbf{G}_1\mathbf{X}. \tag{2}$$

Thus, it looks like it would be possible to find some approximate solutions of the initial integral equation using some appropriate L_2 bases through the simple matrix algebra. However, not everyone L_2 basis suits for this purpose. The integral kernel of the Faddeev equation includes the fixed-pole singularities and also the complicated moving singularities above the three-body breakup threshold. Just these singularities correspond to the proper boundary conditions in coordinate space and provide the correct physical solution of the Faddeev equations, but a construction of the appropriate basis for the projection of such kernels is highly non-trivial problem. Another key problem here is a calculation of matrix elements for v_1, P and especially for G_1 operators in the chosen basis, that can appear, in general, rather cumbersome task. In this point the appropriate stationary wave-packet basis helps to overcome all the above difficulties and formulate the matrix equations whose solutions can really approximate the solutions of the initial integral equations. Such a basis will be demonstrated to provide a convenient analytical diagonal representation for the three-body channel resolvent matrix $\mathbf{G}_1$ and, on the other hand, this basis covers a sufficiently wide functional L_2 space to provide well converged results.

[2] As far as the present authors are aware this is the first precise fully L_2 approximated solution for the Faddeev equation above the three-body threshold.

The channel Hamiltonian H_1 is the direct sum of two subHamiltonians corresponding to the system motion along two independent Jacoby coordinates:

$$H_1 \equiv h_1 \oplus h_0, \tag{3}$$

where subHamiltonian h_1 defines the NN subsystem motion (including interaction v_1) and subHamiltonian h_0 corresponds to the free motion of the third nucleon relatively the NN subsystem center of mass. Now let's define two sets of momentum bins $[p_{m-1}, p_m]_{m=1}^{M}$ and $[q_{n-1}, q_n]_{n=1}^{N}$ corresponding to the continuum discretizations for subHamiltonians h_1 and h_0. The (two-body) stationary wave-packet bases (WPB) are defined as integrals of exact continuum wave functions $|\psi_p\rangle$ and $|\psi_{0q}\rangle$ of subHamiltonians h_1 and h_0 over the respective momentum bins:

$$|z_m\rangle = \frac{1}{\sqrt{b_m}} \int_{p_{m-1}}^{p_m} \mathrm{d}p |\psi_p\rangle, \quad |y_n\rangle = \frac{1}{\sqrt{d_n}} \int_{q_{n-1}}^{p_n} \mathrm{d}q |\psi_{0q}\rangle, \tag{4}$$

where $b_m \equiv p_m - p_{m-1}$ and $d_n \equiv q_n - q_{n-1}$ are bin widths. Now, the three-body WPB states $|S_{ij}\rangle$ are defined just as products of two-body wave-packet states $|z_i\rangle$ (including the bound state wave function $|z_0\rangle$) and $|y_j\rangle$:

$$|S_{ij}\rangle \equiv |z_i, y_j\rangle. \tag{5}$$

We omit here partial wave indices for the sake of simplicity. The properties of the wave-packet sets $|z_i\rangle$ and $|y_j\rangle$ have been investigated in detail in refs. [20, 21, 22, 23]. In particular, the very useful property of such a packet basis is that the matrices for the projected resolvents of subHamiltonians $g_1(E) = (E + \mathrm{i}0 - h_1)^{-1}$ and $g_0 = (E + \mathrm{i}0 - h_0)^{-1}$ are diagonal and defined by a simple analytical expressions depending only on the spectrum discretization parameters. This property of WPB allows us to construct the f.-d. analytical diagonal representation for the channel resolvent $G_1(E)$, which is a convolution of two-body resolvents g_1 and g_0.

Indeed, the exact three-body channel resolvent can be written [21] as a sum of two terms $G_1(E) = G_1^{\mathrm{BC}}(E) + G_2^{\mathrm{CC}}$, where the bound-continuum part has the form:

$$G_1^{\mathrm{BC}}(E) = \int_0^\infty \mathrm{d}q \frac{|z_0, \psi_{0q}\rangle\langle z_0, \psi_{0q}|}{E + \mathrm{i}0 - \epsilon_0 - \frac{3q^2}{4m}}, \tag{6}$$

and ϵ_0 is the binding energy for the (single) NN bound state. The continuum-continuum part takes the form:

$$G_1^{\mathrm{CC}}(E) = \int_0^\infty \mathrm{d}p \int_0^\infty \mathrm{d}q \frac{|\psi_p, \psi_{0q}\rangle\langle\psi_p, \psi_{0q}|}{E + \mathrm{i}0 - \frac{p^2}{m} - \frac{3q^2}{4m}}. \tag{7}$$

Now let's construct a projection of the exact channel resolvent onto the three-body WPB. The following analytical formulas for the diagonal f.-d. projection of G_1 can then be found:

$$\mathbf{G}_1^{\mathrm{BC}} = \sum_j G_{0j}^{BC} |z_0, y_j\rangle\langle z_0, y_j|,$$
$$\mathbf{G}_1^{\mathrm{CC}} = \sum_{i\neq 0, j} G_{ij}^{CC} |z_i, y_j\rangle\langle z_i, y_j|, \tag{8}$$

where the matrix elements $G_{oj}^{\rm BC}$ and $G_{ij}^{\rm CC}$ in eq. (8) are defined as integrals over the respective momentum bins:

$$G_{0j}^{BC} = \frac{1}{d_j}\int_{q_{j-1}}^{q_j} \frac{{\rm d}q}{E+{\rm i}0-\epsilon_0-\frac{3q^2}{4m}}, \qquad (8a)$$

$$G_{ij}^{CC} = \frac{1}{d_i d_j}\int_{p_{i-1}}^{p_i}\int_{q_{j-1}}^{q_j} \frac{{\rm d}p{\rm d}q}{E+{\rm i}0-\frac{p^2}{m}-\frac{3q^2}{4m}}. \qquad (8b)$$

These matrix elements depend, in general, on the spectrum partition parameters (i.e. p_i and q_j values). However we found when the wave-packet expansions of the three-body amplitude is convergent the final result turns out to be *independent* upon the particular spectral partition parameters. The integrals in eqs.(8a) and (8b) are analytically tractable that gives a simple analytical f.-d. representation for the three-body channel resolvent G_1. Such an analytical representation is main feature of the wave-packet approach since it allows to simplify solution of the general three-body scattering problem drastically.

Now the key question arises: how to construct practically the above wave-packet basis. The free packets $|y_n\rangle$ corresponding to the free motion of third nucleon relatively the NN subsystem c.m. take in the momentum representation the form of simple step-like functions:

$$\langle q|y_j\rangle = \frac{\theta(q-q_{j-1})-\theta(q-q_j)}{\sqrt{d_j}}, \qquad (9)$$

where $\theta(x)$ is the Heaviside function.

The scattering wave packets $|z_i\rangle$ describing the scattering in the NN two-body subsystem can be very well approximated by pseudostates $|\tilde{z}_i\rangle$ obtained from the diagonalization of the subHamiltonian h_1 in some appropriate L_2 basis [20]. In the present work we use for this diagonalization a free wave-packet basis $|x_k\rangle$ corresponding to the free NN motion. Thus, we solve the two-body variational problem directly on the free WPB and as a result obtain a set of variational functions

$$|\tilde{z}_i\rangle = \sum_{k=0}^{M} O_{ik}|x_k\rangle, \qquad i=0,\ldots,M, \qquad (10)$$

the first of which (for the problem in question) is the wavefunction of the bound state (deuteron) and other ones are very good approximations for the exact scattering packets.

In the Fig. 1 the coordinate-space behavior of some from the first 50 variational functions (including the deuteron) is shown. It is clear that the free packet basis allows to approximate the respective scattering wave functions up to a very far asymptotic region (in the Figure the functions $\tilde{z}_i(r)$ are given at $r<80$ fm, but actually they coincide with exact scattering wave packets up to $r\sim 1000$ fm). This long-range behavior of the basis functions plays a crucial role in the three-body scattering, especially above the breakup threshold, because it

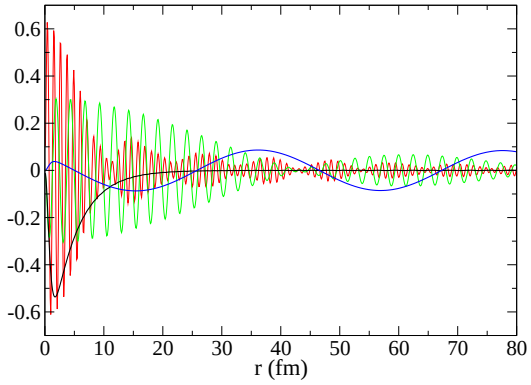

FIG. 1: (Color online) Bound state (solid curve) and several interaction wave packets (different dashed lines) for the MT III potential constructed from the free momentum packets in the coordinate space.

provides a proper overlapping between basis functions in different Jacoby-coordinate sets. It should be mentioned that in our previous calculations [21] we used Gaussian basis to approximate the interaction packets in the whole space and so the wrong long-range behavior of the basis functions did not allow us to obtain well converged results above the break-up threshold (while for the smaller energies the Gaussian approximation works well)[3].

Besides, the momentum lattice basis is very convenient to find the matrix elements of the permutation operator P. Using approximation (10) for the scattering packets $|z_i\rangle$, these matrix elements can be expressed in the form:

$$P_{ij,i'j'} = \langle z_i y_j|P|z_{i'}y_{j'}\rangle \approx \sum_{kk'} O_{ik}O^*_{i'k'}P^0_{kj,k'j'}, \qquad (11)$$

where $P^0_{kj,k'j'}\equiv\langle x_k y_j|P|x_{k'}y_{j'}\rangle$ is the permutation matrix elements taken on the two-dimensional free wave packets (for a two-dimensional lattice). Using hyperspherical momentum coordinates, the calculation of $P^0_{kj,k'j'}$ can be reduced to a one-dimensional numerical integration over hypermomentum p^2+q^2. The technique of this calculation will be given in detail elsewhere. It should be stressed here that this is one of the key points for the whole our approach. In fact, to solve two-dimensional Faddeev equations by conventional methods [4] one needs (due to the appearance of permutation operator P in the integral kernel) to use a very time-consuming two- and three-dimensional interpolations (many thousands or even millions of such interpo-

[3] It should be noted the free packet basis (i.e. the step-like functions in the momentum space) is, of course, not optimal for calculation of bound states. E.g. in our case only 20 Gaussian functions are necessary to obtain $E_b=-2.225$ MeV and ca. 100 step-like functions are required to reach the same precise bound energy value. However very good approximation of scattering wave functions in two-body subsystems is the decisive factor here.

lations) at each iteration step to find the solution in the initial Jacoby set from the "rotated" (by the permutation P) Jacoby sets. So, such numerous multi-dimensional interpolations at each step take a big portion of computational time in practical solutions of three-body integral equations. When solving the four-body Yakubovsky equations the dimension and number of the above each step interpolations gets even higher. Thus, the wave-packet approach allows to avoid such multi-dimensional interpolations.

After solving the matrix eq. (2), the on-shell elastic amplitude $A_{\rm el}(E)$ in wave-packet approximation can be found as a diagonal (on-shell) matrix element of X-matrix (which is a solution of the matrix equation (2)):

$$A_{\rm el}(E) \approx \frac{2m}{3q_0} \frac{X_{0n_0,0n_0}}{d_{n_0}}, \qquad (12)$$

where index n_0 being denote the singular q-bin to which the on-shell momentum $q_0 = \sqrt{\frac{4}{3}m(E-\epsilon_0)}$ belongs: $q_0 \in (q_{n_0-1}, q_{n_0})$. Let's notice that in order to find the elastic amplitude according to eq. (12), one needs to solve one linear equation only just for one column $X_{mn,0n_0}$, but not to do a full matrix inversion in eq. (2).

3. Numerical results. To illustrate the accuracy and effectiveness of the proposed wave-packet technique we calculated the real phase shifts and inelasticity parameters for the three-body elastic $n-d$ scattering in the quartet and doublet S-wave channels with the model Malfliet-Tjon NN potential MT-III. The results of these calculations are shown in Figs. 2 and 3 for the spin-quartet and in Figs. 4 and 5 for the spin-doublet channels respectively.

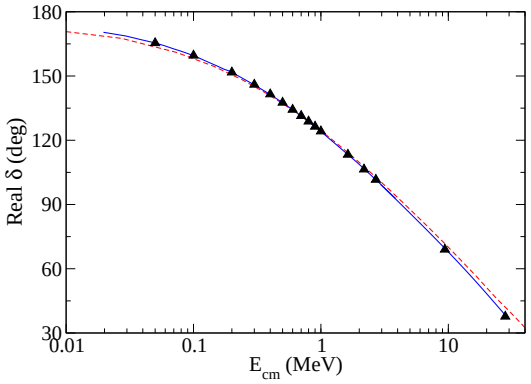

FIG. 2: (Color online) The energy dependence of the real phase shift for S-wave quartet nd scattering calculated by means of the momentum-packet discretized Faddeev equation at different dimensions $M \times N$ of the lattice basis: 100×100 (dashed curve), 200×200 (solid curve). Results of the direct Faddeev equation solution from ref.[7, 8] are marked as ▲.

In the case of doublet scattering one has the system of two matrix equations instead of one matrix equation (2) where two amplitudes correspond to two possible spin

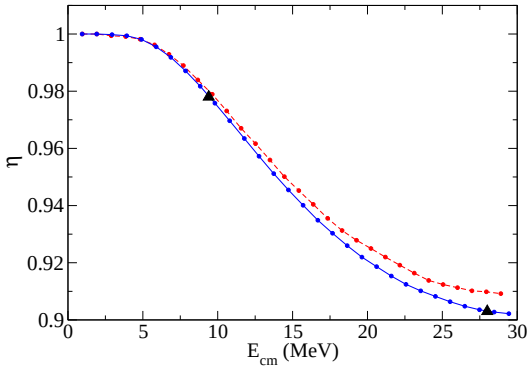

FIG. 3: (Color online) The same as in Fig. 2 but for the inelasticity parameter η.

states (triplet and singlet) of the NN subsystem. To check the accuracy of the method we have compared our results with the previous benchmark calculation results from ref. [7] (below the deuteron breakup threshold) and ref. [8] (above the deuteron breakup threshold) The exact parameters of the NN potential are taken from ref. [8].

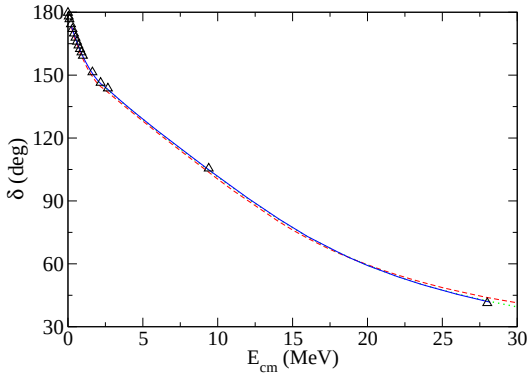

FIG. 4: (Color online) The energy dependence of the real phase shift for the S-wave doublet nd scattering calculated by means of momentum-packet discretized Faddeev equation at different dimensions $M \times N$ of the lattice basis: $(50+50) \times 50$ (dashed curve), $(80+80) \times 80$ (dotted curve) and $(100+100) \times 100$ (solid curve). Results of the direct Faddeev equation solution from ref.[7, 8] are marked as △.

As it is seen from the Figs. 2-5 the wave-packet discretization technique for the three-body continuum works successfully for the general three-body scattering problem both below and above breakup threshold. Thus, at the first time we have solved the three-body scattering problem above the breakup threshold using only f.-d. approximation of the L_2-type for the Faddeev kernel. Just the use of the momentum-lattice basis allowed us to achieve a good convergence and accuracy on this way. It is interesting to remark that although the quartet case seems to be simpler from the first glance (one equation and the inelasticity is less than that in the doublet case)

it turns out to be more difficult numerical problem (the larger basis is needed for convergence) for the wave packet discretization approach.

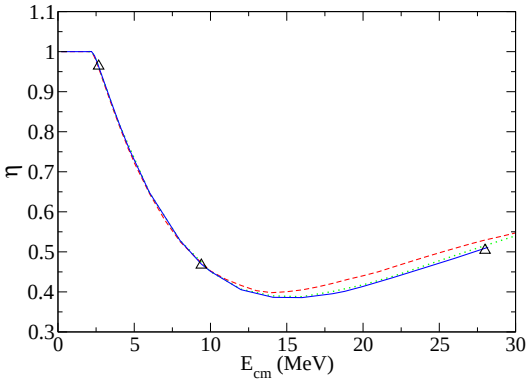

FIG. 5: (Color online) The same as in Fig. 4 but for the inelasticity parameter η.

4. Conclusion. Let's briefly outline here the most important points of this study. For the first time the three-body scattering problem in the Faddeev framework above the breakup threshold has been successfully solved in the three-body L_2 basis representation using the lattice approximation scheme (which is the technique of the three-body continuum discretization). The success and advantages of the lattice approach are related to the following distinctive features.

(i) The explicit analytical f.-d. approximation for the three-body channel resolvent G_1 allows to reduce initial integral Faddeev equation to the matrix one that can be solved directly on the real energy axis.

(ii) The scattering wave packets (corresponding to the NN interaction) can be approximated by pseudostates of the two-body NN subHamiltonian matrix in the free wave-packet basis, which allows to avoid calculation of the two-body t-matrix and obtain explicitly matrix elements of the permutation operator P that includes overlapping between wave-packet basis states of the different three-body channel Hamiltonians.

(iii) This convenient closed form for the matrix elements of the permutation operator P in the WPB also makes it possible to avoid completely very time-consuming multi-dimensional interpolations of the iterated kernels which are usually assist in conventional techniques of the Faddeev equation numerical integration in the momentum space.

(iv) The very long-range type of the wave-packet functions (non-vanishing at distances $\sim$ 1000 fm) allows to approximate properly the overlapping between basis states in different Jacoby coordinate sets. This leads to the proper asymptotic behavior of the solutions along different Jacoby coordinates, which couldn't be provided by means of conventionally used short-range type L_2 bases.

Besides, this long-range behavior of the wave-packet basis functions looks also very promising for the proper incorporation of the long-range Coulomb interaction in the treatment of the few-nucleon scattering. Our further investigations are pointed at this purpose.

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